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A microscopic derivation of the Born–Huang relations between the atomic force constants

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SUMMARY

M. Born and K. Huang have derived a general relation [1, 2] between the elastic constants and the atomic force constants by considering long acoustic waves in an infinitely large lattice. The symmetry properties of the elastic constants lead to certain linear relations between the atomic force constants that could not be predicted from a microscopic treatment.

It is shown here that by taking the finite extension of the lattice into account the Born–Huang relations readily follow in the microscopic treatment.

1. Introduction

According to Hooke's law the relation between the stress tensor, $\sigma_{\alpha\beta}$, and the strain tensor, $\varepsilon_{\alpha\beta}$, is linear,

$$\sigma_{\alpha\beta} = \sum_{\mu\nu} c_{\alpha\beta,\mu\nu}\, \varepsilon_{\mu\nu}. \tag{1.1}$$

The elastic constants $c_{\alpha\beta,\mu\nu}$ have the symmetry properties

$$c_{\alpha\beta,\mu\nu} = c_{\beta\alpha,\mu\nu} = c_{\mu\nu,\alpha\beta}. \tag{1.2}$$

The subgroup of the permutation group which leaves $c_{\alpha\beta,\mu\nu}$ invariant will be called G and instead of (1.2) we write

$$c_{\alpha\beta,\mu\nu} \in G. \tag{1.3}$$

There are in general 21 independent elastic constants.

When the solid is under initial strain a small change in the stress tensor may still be linear in the changes of the strain tensor but the constants of proportionality, the "linearized elastic constants", no longer belong to G (see appendix).

The microscopic theory of elasticity is built on the concept of interatomic forces. These are derived from an atomic potential energy usually taken in the adiabatic approximation. The second derivatives of the potential are called force constants. Born and Huang have derived a relation between the force constants and the elastic constants by comparing the microscopic equation for long waves with the equation for the acoustic waves as given by the theory of elasticity.[1]

We conclude this introduction with a brief survey of the Born-Huang results and references are given to equations in their book [4].

The atomic potential Φ is a function of the atomic coordinates $x_\alpha\begin{pmatrix} l \\ k \end{pmatrix}$, where α is a cartesian index, l indicates a lattice cell and k a specific atom of the cell. They consider small changes of the coordinates from $\bar{x}\begin{pmatrix} l \\ k \end{pmatrix} = \sum_{r=1}^{3} l_r \bar{a}_r + \bar{x}(k)$ corresponding to equilibrium positions, to $\bar{x}\begin{pmatrix} l \\ k \end{pmatrix} + \bar{u}\begin{pmatrix} l \\ k \end{pmatrix}$. The corresponding change in the potential is

$$\Delta\Phi = \tfrac{1}{2} \sum_{\substack{l l' k k' \\ \alpha\beta}} \Phi_{\alpha\beta}\begin{pmatrix} l\,l' \\ k\,k' \end{pmatrix} u_\alpha\begin{pmatrix} l \\ k \end{pmatrix} u_\beta\begin{pmatrix} l' \\ k' \end{pmatrix} + \dots, \tag{1.4}$$

where the quantities $\Phi_{\alpha\beta}\begin{pmatrix} l\,l' \\ k\,k' \end{pmatrix}$ are called force constants. As they consider an infinite lattice the absence of the first order terms in $\Delta\Phi$ does not exclude the possibility of a finite strain. On account of the lattice symmetry

$$\Phi_{\alpha\beta}\begin{pmatrix} l\,l' \\ k\,k' \end{pmatrix} = \Phi_{\alpha\beta}\begin{pmatrix} l+l'' & l'+l'' \\ k & k' \end{pmatrix}.$$

It is convenient to use the notations

$$\Phi_{\alpha\beta}\begin{pmatrix} l \\ k\,k' \end{pmatrix} = \Phi_{\alpha\beta}\begin{pmatrix} l\,0 \\ k\,k' \end{pmatrix}$$

and

$$\bar{x}\begin{pmatrix} l \\ k\,k' \end{pmatrix} = \bar{x}\begin{pmatrix} l\,0 \\ k\,k' \end{pmatrix} = \bar{x}\begin{pmatrix} l \\ k \end{pmatrix} - \bar{x}\begin{pmatrix} 0 \\ k' \end{pmatrix}.$$

The method of "long waves" gives (compare eq. 28.7),

$$S_{\alpha\gamma,\beta\lambda} + S_{\alpha\lambda,\beta\gamma} = 2\,[\alpha\beta,\gamma\lambda] + (\alpha\gamma,\beta\lambda) + (\alpha\lambda,\beta\gamma). \tag{1.5}$$

Here $S_{\alpha\gamma,\beta\lambda}$ is a coefficient in the elastic energy density (4.2) and we show in the appendix that it also is a linearized elastic constant. The symmetry properties of the coefficients in (4.2) are

$$S_{\alpha\beta} = S_{\beta\alpha}, \tag{1.6}$$

$$T_{\alpha\gamma,\beta\lambda} \in G, \tag{1.7}$$

where

$$T_{\alpha\gamma,\beta\lambda} = S_{\alpha\gamma,\beta\lambda} - \delta_{\alpha\beta}\, S_{\gamma\lambda}. \tag{1.8}$$

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[1] These relations may also be derived by the method of deformation fields [3]. Notice that the article [1] by Begbie and Born contains some mistakes which were corrected in the article [2] by Huang.

The terms of the right member of equation (1.5) are (v_a = volume of lattice cell),

$$[\alpha\beta, \gamma\lambda] = -\frac{1}{2 v_a} \sum_{l k k'} \Phi_{\alpha\beta}\begin{pmatrix} l \\ k\,k' \end{pmatrix} x_\gamma \begin{pmatrix} l \\ k\,k' \end{pmatrix} x_\lambda \begin{pmatrix} l \\ k\,k' \end{pmatrix} \tag{1.9}$$

and $(\alpha\gamma, \beta\lambda)$ which is a complicated non-linear expression in the force constants. When the magnitude of the vector l increases the force constants $\Phi_{\alpha\beta}\begin{pmatrix} l \\ k\,k' \end{pmatrix}$ rapidly tend to zero. The lattice sum (1.9) is expected to converge for all solids except the piezoelectric ones.

The microscopic treatment of the infinite lattice shows that

$$[\alpha\beta, \gamma\lambda] = [\beta\alpha, \gamma\lambda] = [\alpha\beta, \lambda\gamma], \tag{1.10}$$

$$(\alpha\beta, \gamma\lambda) \in G. \tag{1.11}$$

Using (1.8) we may rewrite equation (1.5),

$$[T_{\alpha\gamma,\beta\lambda} - (\alpha\gamma, \beta\lambda)] + [T_{\alpha\lambda,\beta\gamma} - (\alpha\lambda, \beta\gamma)] = 2\{[\alpha\beta, \gamma\lambda] - \delta_{\alpha\beta} S_{\gamma\lambda}\}. \tag{1.12}$$

The left member is invariant when we permute $\alpha\gamma\beta\lambda$ into $\gamma\alpha\lambda\beta$. Demanding this invariance of the right member we obtain new relations which together with eq. (1.10) may be writen

$$e_{\alpha\beta,\gamma\lambda} \in G, \tag{1.13}$$

where

$$e_{\alpha\beta,\gamma\lambda} = [\alpha\beta, \gamma\lambda] - \delta_{\alpha\beta} S_{\gamma\lambda}. \tag{1.14}$$

The tensor

$$[\alpha\beta, \gamma\lambda] = \tfrac{1}{2}[\delta_{\alpha\beta} S_{\gamma\lambda} - \delta_{\gamma\lambda} S_{\alpha\beta}] + \tfrac{1}{2}[\delta_{\alpha\beta} S_{\gamma\lambda} + \delta_{\gamma\lambda} S_{\alpha\beta}] + e_{\alpha\beta\gamma\lambda}$$

has 26 independent components. This is easily seen since the first parenthesis on the right hand side may be described by 5 parameters and the remaining terms by 21 parameters.

The relations (1.10) show that $[\alpha\beta, \gamma\lambda]$ has at most 36 independent components and thus the properties of the coefficients $S_{\alpha\beta,\gamma\lambda}$ infer $36 - 26 = 10$ new linear relations between the force constants. These are the "Born–Huang relations" (28.32)–(28.35).

2. Invariance relations in a finite lattice

We first derive some relations that are valid for an arbitrary system of N particles interacting via a potential $\Phi(\bar{x}_1, \bar{x}_2, \dots \bar{x}_N)$. We use a simpler notation than in the preceding section. A Greek index will specify the cartesian component and a Latin index the particle, for example; $(\bar{x}_i)_\alpha = x_{i\alpha}$. The derivatives are written

$$\Phi_{i\alpha} = \frac{\partial \Phi}{\partial x_{i\alpha}}; \quad \Phi_{ij\alpha\beta} = \frac{\partial^2 \Phi}{\partial x_{i\alpha} \partial x_{j\beta}}; \quad \text{etc.} \tag{2.1}$$

We immediately have the relation

$$\Phi_{ij\alpha\beta} = \Phi_{ji\beta\alpha}. \tag{2.2}$$

The potential is invariant under translations and rigid rotations,

$$\Phi(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_N) = \Phi(\bar{x}_1 + \bar{a}, \bar{x}_2 + \bar{a}, \ldots, \bar{x}_N + \bar{a}) = \Phi(P\bar{x}_1, P\bar{x}_2, \ldots, P\bar{x}_N), \tag{2.3}$$

where P is an orthogonal 3×3 matrix.

Taking a partial derivate of (2.3) we obtain,

$$\Phi_{i\alpha}(\bar{x}_1, \ldots, \bar{x}_N) = \Phi_{i\alpha}(\bar{x}_1 + \bar{a}, \ldots, \bar{x}_N + \bar{a}) = \sum_{\mu} \Phi_{i\mu}(P\bar{x}_1, \ldots, P\bar{x}_N)\, P_{\mu\alpha}. \tag{2.4}$$

We make a Taylor expansion of (2.3) and (2.4) in the components of $\bar{a}$,

$$\Phi(\bar{x}_1, \ldots) = \Phi(\bar{x}_1, \ldots) + \sum_{i\alpha} \Phi_{i\alpha} a_\alpha + \ldots,$$

$$\Phi_{i\alpha}(\bar{x}_1, \ldots) = \Phi_{i\alpha}(\bar{x}_1, \ldots) + \sum_{j\beta} \Phi_{ij\alpha\beta} a_\beta + \ldots.$$

Hence

$$\sum_i \Phi_{i\alpha} = \sum_j \Phi_{ij\alpha\beta} = 0. \tag{2.5}$$

When P corresponds to a small rotation it may be written

$$P_{\alpha\beta} = \delta_{\alpha\beta} + \omega_{\alpha\beta} + \ldots; \quad \omega_{\alpha\beta} = -\omega_{\beta\alpha}. \tag{2.6}$$

We make a Taylor expansion of (2.3) and (2. 4) in $\omega_{\alpha\beta}$,

$$\Phi(\bar{x}_1, \ldots) = \Phi(\bar{x}_1, \ldots) + \sum_{i\alpha\beta} \Phi_{i\alpha} x_{i\beta}\, \omega_{\alpha\beta} + \ldots,$$

$$\begin{aligned}\Phi_{i\alpha}(\bar{x}_1, \ldots) &= \sum_{\mu} (\delta_{\mu\alpha} + \omega_{\mu\alpha} + \cdots)\Big(\Phi_{i\mu}(\bar{x}_1, \ldots) + \sum_{j\beta\nu} \Phi_{ij\mu\nu} x_{j\beta}\, \omega_{\nu\beta} + \cdots\Big)\\ &= \Phi_{i\alpha}(\bar{x}_1, \ldots) + \sum_{j\beta\nu} \Phi_{ij\alpha\nu} x_{j\beta}\, \omega_{\nu\beta} + \sum_{\mu} \Phi_{i\mu}\, \omega_{\mu\alpha} + \ldots.\end{aligned}$$

Hence

$$\sum_i \Phi_{i\alpha} x_{i\beta} = \sum_i \Phi_{i\beta} x_{i\alpha}, \tag{2.7}$$

$$\sum_j \Phi_{ij\alpha\nu} x_{j\beta} + \Phi_{i\nu}\, \delta_{\alpha\beta} = \sum_j \Phi_{ij\alpha\beta} x_{j\nu} + \Phi_{i\beta}\, \delta_{\alpha\nu}. \tag{2.8}$$

Introducing the quantities

$$T_{\alpha\beta} = \frac{1}{V} \sum_i \Phi_{i\alpha} x_{i\beta}, \tag{2.9}$$

$$d_{\alpha\mu\nu\beta} = \frac{1}{V} \sum_{ij} \Phi_{ij\alpha\beta} x_{i\mu} x_{j\nu}, \tag{2.10}$$

where V is the volume of the convex polyhedron spanned by the particles, we obtain from (2.7)

$$T_{\alpha\beta} = T_{\beta\alpha} \tag{2.11}$$

and from (2.8) after multiplying by $x_{i\mu}$ and summing over i

$$d_{\alpha\mu\beta\nu} + \delta_{\alpha\beta}\, T_{\mu\nu} = d_{\alpha\mu\nu\beta} + \delta_{\alpha\nu}\, T_{\beta\mu}. \tag{2.12}$$

From (2.2) and the definition (2.10) of $d_{\alpha\mu\nu\beta}$ we find

$$d_{\alpha\mu\nu\beta} = d_{\beta\nu\mu\alpha}. \tag{2.13}$$

The equations (2.12) and (2.13) may be combined to

$$D_{\alpha\mu\nu\beta} \in G, \tag{2.14}$$

where

$$D_{\alpha\mu\nu\beta} = d_{\alpha\mu\nu\beta} - \delta_{\alpha\beta}\, T_{\mu\nu}. \tag{2.15}$$

We now specialize our results to the case when the particles form a space lattice. In the previous notation the positions are

$$\bar{x}\begin{pmatrix} l \\ k \end{pmatrix} = \sum_{r=1}^{3} l_r \bar{a}_r + \bar{x}(k); \quad 1 \leqslant l_r \leqslant N_r; \quad 1 \leqslant k \leqslant M. \tag{2.16}$$

From (2.2), (2.5), (2.9) and (2.10) we have

$$\Phi_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} = \Phi_{\beta\alpha}\begin{pmatrix} l'\, l \\ k'\, k \end{pmatrix}, \tag{2.17}$$

$$\sum_{lk} \Phi_{\alpha}\begin{pmatrix} l \\ k \end{pmatrix} = \sum_{l'k'} \Phi_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} = 0. \tag{2.18}$$

$$T_{\alpha\beta} = \frac{1}{V} \sum_{lk} \Phi_{\alpha}\begin{pmatrix} l \\ k \end{pmatrix} x_{\beta}\begin{pmatrix} l \\ k \end{pmatrix}, \tag{2.19}$$

$$d_{\alpha\mu\nu\beta} = \frac{1}{V} \sum_{ll'kk'} \Phi_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} x_{\mu}\begin{pmatrix} l \\ k \end{pmatrix} x_{\nu}\begin{pmatrix} l' \\ k' \end{pmatrix}. \tag{2.20}$$

Using (2.18) we obtain the identity

$$\sum_{ll'kk'} \Phi_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} x_{\mu}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} x_{\nu}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} = -\sum_{ll'kk'} \Phi_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} \left\{ x_{\mu}\begin{pmatrix} l \\ k \end{pmatrix} x_{\nu}\begin{pmatrix} l' \\ k' \end{pmatrix} + x_{\nu}\begin{pmatrix} l \\ k \end{pmatrix} x_{\mu}\begin{pmatrix} l' \\ k' \end{pmatrix} \right\}. \tag{2.21}$$

The right member is equal to $-V(d_{\alpha\mu\nu\beta} + d_{\alpha\nu\mu\beta})$. The left member can be written

$$\sum_{l'}^{l' \in L} \sum_{l''}^{(l'+l'') \in L} \sum_{kk'} \Phi_{\alpha\beta}\begin{pmatrix} l'+l''\; l' \\ k \quad k' \end{pmatrix} x_{\mu}\begin{pmatrix} l'' \\ k\, k' \end{pmatrix} x_{\nu}\begin{pmatrix} l'' \\ k\, k' \end{pmatrix}. \tag{2.22}$$

The notations $l' \in L$ and $(l' + l'') \in L$ indicate that the vector components satisfy the conditions in (2.16).

If the lattice is infinite then $\Phi_{\alpha\beta}\begin{pmatrix} l'+l''\, l' \\ k\, k' \end{pmatrix} = \Phi_{\alpha\beta}\begin{pmatrix} l'' \\ k\, k' \end{pmatrix}$ and the summation in (2.22) over l'', k and k' gives $-2v_a[\alpha\beta,\mu\nu]$ according to equation (1.9). In a finite lattice this only represents an approximation which becomes better the larger the distance between the point $\bar{x}(l')$ and the boundary of the lattice. Under certain[1] conditions we obtain

$$-2v_a[\alpha\beta,\ \mu\nu]\,N + O(N^{\frac{2}{3}}) = -V\,[d_{\alpha\mu\nu\beta} + d_{\alpha\nu\mu\beta}], \tag{2.23}$$

where $N = N_1 N_2 N_3$ is the number of lattice cells. Since we consider N as very large we write

$$[\alpha\beta,\ \mu\nu] = \tfrac{1}{2}\,(d_{\alpha\mu\nu\beta} + d_{\alpha\nu\mu\beta}) \tag{2.24}$$

neglecting the term $\theta(N^{-\frac{1}{3}})$, From (2.15) and (2.24) we obtain

$$f_{\alpha\beta\mu\nu} = \tfrac{1}{2}\,(D_{\alpha\mu\nu\beta} + D_{\alpha\nu\mu\beta}), \tag{2.25}$$

where

$$f_{\alpha\beta\mu\nu} = [\alpha\beta,\ \mu\nu] - \delta_{\alpha\beta}\,T_{\mu\nu}. \tag{2.26}$$

Since $D_{\alpha\mu\nu\beta} \in G$ and $f_{\alpha\beta\mu\nu} = f_{\beta\alpha\mu\nu} = f_{\alpha\beta\nu\mu}$ we obtain from (2.25), (compare the derivation of (1.13)),

$$f_{\alpha\beta\mu\nu} \in G. \tag{2.27}$$

This shows that $[\alpha\beta,\ \mu\nu]$ obeys the Born–Huang relations.

The essential steps in the proof are

(i) rotational invariance of Φ gives $D_{\alpha\mu\nu\beta} \in G$;

(ii) neglecting certain terms associated with the surface gives a relation between $[\alpha\beta,\ \mu\nu]$ and $D_{\alpha\mu\nu\beta}$, equation (2.25).

3. Remarks

The results in the previous section were obtained by considering a finite lattice whose dimensions became infinitely large instead of introducing the infinite lattice from the outset (compare the recent work by E. Stern [5]). It is convenient to denote quantities referring to the limit case of an infinite lattice with a superscript ^{0}.

We observe that in the derivation of the Born–Huang relations we only used the translational symmetry of the lattice. Then we have $\sum_k \Phi^0_\alpha\begin{pmatrix} l \\ k \end{pmatrix} = 0$ but not necessarily $\Phi^0_\alpha\begin{pmatrix} l \\ k \end{pmatrix} = 0$, which represents a slight extension of the validity of the Born-Huang relations.

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[1] The difference between the force constants in a finite and an infinite lattice must decrease sufficiently rapid with the distance from the boundary, and the lattice sum in (1.9) must converge sufficiently fast. The sufficiency conditions are however very weak. Thus if, for example, in (1.9) the sum over k, k' and l satisfying $|\bar{x}(l)| < r$ gives a remainder term smaller than $r^{-\varepsilon}$, $\varepsilon > 0$ they are fulfilled.

We further note that the present technique makes it possible to obtain the relation between the elastic constants and the force constants by considering *a homogeneous deformation* instead of long waves. This has the twin virtue of allowing the complete derivation to be made with a finite lattice and being simpler than the method of long waves. We give a sketch of the derivation.

Consider a small homogeneous deformation from the equilibrium positions

$$\bar{x}\begin{pmatrix} l \\ k \end{pmatrix} = \sum_r l_r \bar{a}_r + \bar{x}(k) \quad \text{to} \quad \bar{x}\begin{pmatrix} l \\ k \end{pmatrix} + \bar{u}\begin{pmatrix} l \\ k \end{pmatrix},$$

where

$$u_\alpha\begin{pmatrix} l \\ k \end{pmatrix} = \sum_\beta u_{\alpha\beta}\, x_\beta\begin{pmatrix} l \\ k \end{pmatrix} + u_\alpha(k), \quad u_{\alpha\beta} \to 0. \tag{3.1}$$

The vectors $\bar{u}(k)$ are determined from the condition that

$$\sum_{\beta l' k'} \Phi^0_{\alpha\beta}\begin{pmatrix} l\,l' \\ k\,k' \end{pmatrix} u_\beta\begin{pmatrix} l' \\ k' \end{pmatrix} = 0.$$

The change in the potential Φ becomes,

$$\begin{aligned}\Delta\Phi = {} & \sum_{\substack{l k \\ \alpha\beta}} \Phi_\alpha\begin{pmatrix} l \\ k \end{pmatrix} x_\beta\begin{pmatrix} l \\ k \end{pmatrix} u_{\alpha\beta} + \sum_{\substack{l k \\ \alpha}} \Phi_\alpha\begin{pmatrix} l \\ k \end{pmatrix} u_\alpha(k) \\ & + \tfrac{1}{2} \sum_{\substack{l l' k k' \\ \alpha\beta\mu\nu}} \Phi_{\alpha\beta}\begin{pmatrix} l\,l' \\ k\,k' \end{pmatrix} x_\mu\begin{pmatrix} l \\ k \end{pmatrix} x_\nu\begin{pmatrix} l' \\ k' \end{pmatrix} u_{\alpha\mu}\, u_{\beta\nu} + \tfrac{1}{2} \sum_{\substack{l l' k k' \\ \alpha\beta\mu}} \Phi_{\alpha\beta}\begin{pmatrix} l\,l' \\ k\,k' \end{pmatrix} x_\mu\begin{pmatrix} l \\ k \end{pmatrix} u_{\alpha\mu}\, u_\beta(k') \\ & + \tfrac{1}{2} \sum_{\substack{l l' k k' \\ \alpha\beta}} \Phi_{\alpha\beta}\begin{pmatrix} l\,l' \\ k\,k' \end{pmatrix} u_\alpha(k)\, u_\beta\begin{pmatrix} l' \\ k' \end{pmatrix}. \end{aligned} \tag{3.2}$$

The second and the last terms give under proper conditions contributions proportional to $N^{\frac{2}{3}}$. Neglecting these we have

$$\Delta\Phi = V\{\sum_{\alpha\beta} T_{\alpha\beta}\, u_{\alpha\beta} + \tfrac{1}{2} \sum_{\alpha\beta\mu\nu} [d_{\alpha\mu\nu\beta} + (\alpha\,\mu, \beta\,\nu)]\, u_{\alpha\mu}\, u_{\beta\nu} + \cdots\}, \tag{3.3}$$

where the presence of $(\alpha\,\mu, \beta\,\nu)$ defined in (26.33) may be verified from the relation (26.28) between $u_\alpha(k)$ defined in (26.23) and $u_{\alpha\beta}$ defined in (26.21). (The equations refer to the book by Born and Huang.) From comparison with the elastic energy density (4.2) we have

$$S_{\alpha\beta} = T_{\alpha\beta}, \tag{3.4}$$

$$S_{\alpha\mu,\beta\nu} = d_{\alpha\mu\nu\beta} + (\alpha\,\mu, \beta\,\nu). \tag{3.5}$$

From (2.24) we may solve $d_{\alpha\mu\nu\beta}$ in terms of $[\alpha\,\beta, \mu\,\nu]$,

$$d_{\alpha\mu\nu\beta} = [\alpha\,\beta, \mu\,\nu] + [\alpha\,\nu, \beta\,\mu] - [\alpha\,\mu, \beta\,\nu] + \delta_{\alpha\mu}\, T_{\beta\nu} - \delta_{\alpha\nu}\, T_{\beta\mu}. \tag{3.6}$$

The result is easily checked by aid of (2.25).

From (2.12) and (3.4) we have

$$S_{\mu\nu} = d_{\alpha\mu\nu\alpha} - d_{\alpha\mu\alpha\nu}, \quad \alpha \neq \nu. \tag{3.7}$$

Thus the complete stress tensor is expressed in force constants. We have not however expressed $S_{\mu\nu}$ exclusively in $\Phi^0_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix}$ since the force constants associated with the boundary are involved in a basic way.

The relation (3.7) can be useful if one makes assumptions about the force constants in order to obtain some *model of the solid*. Suppose, for example, that a lattice with cubic symmetry has the *a priori* reasonable property [6]

$$\Phi_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} = A_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix}\left(\frac{V_0}{V}\right)^{2\gamma}, \tag{3.8}$$

where $A_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix}$, V_0 and γ are constants and V is the volume of the solid. According to (3.7) we then have the following expression for the pressure P,

$$P = C_1\left(\frac{V_0}{V}\right)^{2\gamma+\frac{1}{3}}, \quad \frac{\partial P}{\partial V} = C_2 \frac{P}{V}, \tag{3.9}$$

where C_1 and C_2 are constants. The model represents a non-bound solid. This fact which easily follows in the present formalism was not noticed in the original treatment.

If we describe even a modest strain with *a series expansion of* Φ it *may seem strongly divergent* since the $\bar{u}\begin{pmatrix} l \\ k \end{pmatrix}$ easily become thousands of lattice spacings.

Using (2.18), however, we obtain

$$\Phi = \Phi_0 + \sum_{\substack{l \\ k \\ \alpha}} \Phi_\alpha\begin{pmatrix} l \\ k \end{pmatrix} u_\alpha\begin{pmatrix} l\,0 \\ k\,0 \end{pmatrix} + \tfrac{1}{2}\sum_{\substack{l l' \\ k k' \\ \alpha\beta}} \Phi_{\alpha\beta}\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} u_\alpha\begin{pmatrix} l\,0 \\ k\,0 \end{pmatrix} u_\beta\begin{pmatrix} l'\, l \\ k'\, k \end{pmatrix}$$

$$+ \tfrac{1}{6}\sum_{\substack{l l' l'' \\ k k' k'' \\ \alpha\beta\gamma}} \Phi_{\alpha\beta\gamma}\begin{pmatrix} l\, l'\, l'' \\ k\, k'\, k'' \end{pmatrix} u_\alpha\begin{pmatrix} l\,0 \\ k\,0 \end{pmatrix} u_\beta\begin{pmatrix} l'\, l \\ k'\, k \end{pmatrix} u_\gamma\begin{pmatrix} l''\, l \\ k''\, k \end{pmatrix} + \ldots, \tag{3.10}$$

where $u_\alpha\begin{pmatrix} l\, l' \\ k\, k' \end{pmatrix} = u_\alpha\begin{pmatrix} l \\ k \end{pmatrix} - u_\alpha\begin{pmatrix} l' \\ k' \end{pmatrix}$ and the atom $\begin{pmatrix} 0 \\ 0 \end{pmatrix}$ may be taken somewhere in the central part of the solid. This is still not quite convincing because of the factor $u_\alpha\begin{pmatrix} l\,0 \\ k\,0 \end{pmatrix}$. To see that the convergence properties are reasonable we consider a homogeneous deformation. The coefficient of e.g., $u_{\alpha\mu}\, u_{\beta\nu}\, u_{\gamma\lambda}$ is

$$\tfrac{1}{6}\sum_{lk} x_\mu\begin{pmatrix} l \\ k \end{pmatrix} \sum_{l' l'' k' k''} \Phi_{\alpha\beta\gamma}\begin{pmatrix} l\, l'\, l'' \\ k\, k'\, k'' \end{pmatrix} x_\nu\begin{pmatrix} l'\, l \\ k'\, k \end{pmatrix} x_\lambda\begin{pmatrix} l''\, l \\ k''\, k \end{pmatrix} = \tfrac{1}{6}\sum_{lk} x_\mu\begin{pmatrix} l \\ k \end{pmatrix} g_{\alpha\beta\gamma,\nu\lambda}\begin{pmatrix} l \\ k \end{pmatrix}. \tag{3.11}$$

Equation (2.18) gives the identity

$$\sum_{lk} g_{\alpha\beta\gamma,\nu\lambda} \binom{l}{k} = 0. \tag{3.12}$$

The corresponding relation in the limit of an infinite lattice is

$$\sum_{k} g^{0}_{\alpha\beta\gamma,\nu\lambda} \binom{l}{k} = 0. \tag{3.13}$$

If we now split (3.11) into

$$\tfrac{1}{6} \sum_{lk} g_{\alpha\beta\gamma,\nu\lambda} \binom{l}{k} x_\mu(l) + \tfrac{1}{6} \sum_{lk} g_{\alpha\beta\gamma,\nu\lambda} \binom{l}{k} x_\mu(k), \tag{3.14}$$

the first term gives a contribution essentially from the boundary region and both terms are reasonably expected to be proportional to N.

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APPENDIX

Linearized elastic constants

Consider the work done on a solid in a deformation from positions $\bar{x}$ to $\bar{x}+\bar{u}$,

$$\Delta W = \int_S \sum_\alpha F^S_\alpha u_\alpha \, dS + \int_V \sum_\alpha F_\alpha u_\alpha \, dV \tag{4.1}$$

where F^S_α and F_α are the external surface and volume forces corresponding to the positions $\bar{x}$. From the change in the elastic energy density (see, e.g. Born–Huang, p. 241),

$$u = \sum_{\alpha\beta} S_{\alpha\beta} u_{\alpha\beta} + \tfrac{1}{2} \sum_{\alpha\beta\mu\nu} S_{\alpha\mu,\beta\nu} u_{\alpha\mu} u_{\beta\nu} + \ldots, \quad u_{\alpha\beta} = \frac{\partial u_\alpha}{\partial x_\beta}, \tag{4.2}$$

we have

$$\Delta W = \int_V u \, dV = \int_S \sum_{\alpha\beta} S_{\alpha\beta} u_\alpha n_\beta \, dS - \int_V \sum_{\alpha\beta} \frac{\partial S_{\alpha\beta}}{\partial x_\beta} u_\alpha \, dV + \ldots, \tag{4.3}$$

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where n_α are the direction cosines of the surface. The integrations in (4.1) and (4.3) are taken over the positions $\bar{x}$. Since $\bar{u}$ is an arbitrary vector function we have

$$F_\alpha^S = \sum_\beta S_{\alpha\beta} n_\beta. \tag{4.4}$$

$$F_\alpha = -\sum_\beta \frac{\partial S_{\alpha\beta}}{\partial x_\beta}. \tag{4.5}$$

Thus $S_{\alpha\beta}$ is the stress tensor.

Corresponding to the positions $\bar{x}+\bar{u}$ we have slightly different values of F_α^S, $S_{\alpha\beta}$ and n_β,

$$(F_\alpha^S)' = \sum_\beta S'_{\alpha\beta} n'_\beta. \tag{4.6}$$

The difference $S'_{\alpha\beta} - S_{\alpha\beta}$ can be written

$$S'_{\alpha\beta} - S_{\alpha\beta} = \sum_{\mu\nu} C_{\alpha\beta,\mu\nu} u_{\mu\nu} + \dots, \tag{4.7}$$

where

$$C_{\alpha\beta,\mu\nu} = S_{\alpha\beta,\mu\nu} + S_{\alpha\nu}\delta_{\beta\mu} - S_{\alpha\beta}\delta_{\mu\nu} \tag{4.8}$$

may be called linearized elastic constants.

We may also use a stress tensor $S''_{\alpha\beta}$ such that

$$\sum_\beta S'_{\alpha\beta} n'_\beta \, dS' = \sum_\beta S''_{\alpha\beta} n_\beta \, dS. \tag{4.9}$$

The difference $S''_{\alpha\beta} - S_{\alpha\beta}$ can be written

$$S''_{\alpha\beta} - S_{\alpha\beta} = \sum_{\mu\nu} S_{\alpha\beta,\mu\nu} u_{\mu\nu} + \dots . \tag{4.10}$$

Hence the coefficients $S_{\alpha\beta,\mu\nu}$ in the elastic energy density may also be called linearized elastic constants.

These relations may also be obtained from the theory of finite strain as developed by Murnaghan [7] but he does not give the linearized expressions explicitly.

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